Exchangeability, chaos and dissipation in large systems of particles.

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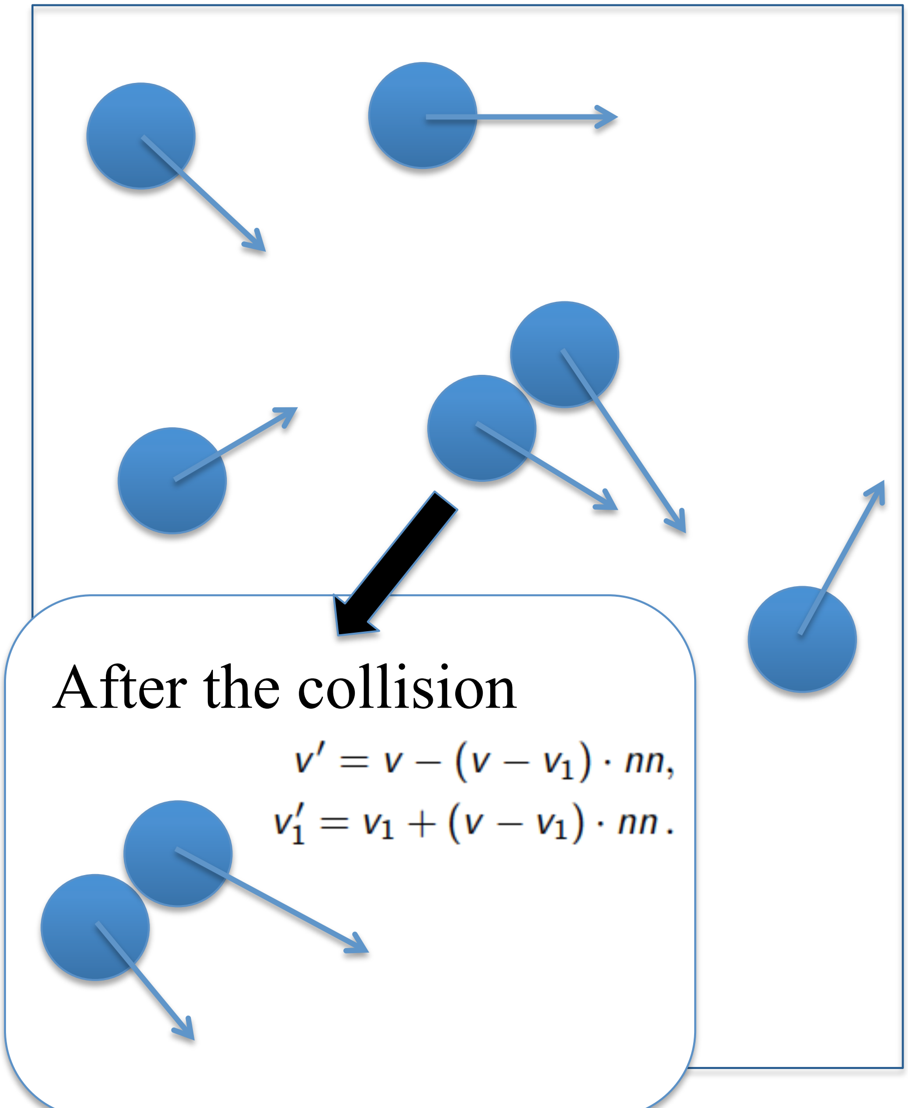
The hard sphere dynamics



The system evolves under the effects of transport and elastic collisions.

- Defined for almost all initial conditions;
- Satisfies the Poincaré recurrence for very large times;
- Strongly unstable.

What can be predicted?

Disorder, also called chaos…
with many different definitions!

<u>Ergodicity</u>

Effect of time averaging

The distribution of positions along a trajectory is generically the uniform distribution on the whole spatial domain.

<u>Decorrelation</u>

Averaging over a large number of particles

Any two tagged particles evolve essentially independently. This leads to preferred configurations (with maximal entropy).

Exchangeability and thermodynamic equilibrium

Maxwell-Boltzmann distribution

« In idealized gases, particles do not interact with one another except for very brief collisions in which they exchange energy and momentum. [...] This means that each particle's state can be considered **independently** from the other particles' state. » (from Wikipedia)

Assuming thermal equilibrium, Maxwell then showed by **symmetry arguments** that the average number of particles in a given single-particle microstate obeys the statistics

$$M_\beta(v) = \left(\frac{\beta}{2\pi}\right)^{d/2} \exp\left(-\frac{\beta}{2}|v|^2\right) .$$

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Ergodicity and invariant measures

For the system of N particles, we expect any invariant measure to **depend only on the energy** (up to a translation of all velocities).

However there are only partial results regarding the **ergodicity of the system** (Sinaï, Chernov, Bunimovitch, Szasz, Simanyi,..)

Theorem

Consider a system of N hard spheres of radius ε and of masses $(m_i)_{1\leq i\leq N}$ in $\mathbb{T}^d$. Then,

- *if $N \leq \max(4, d)$ and $m_i = m$ for all i, the system is ergodic;*
- *if $d = 2$, for all N, the system is ergodic for almost all $(m_i)_{1\leq i\leq N}$.*

Concentration of measure

The central limit theorem then shows that the velocities converge to **independent normal variables** (Poincaré, Borel, De Finetti,...).

In low density regimes, we further have that the spatial **non overlapping condition** disappears in the limit

$$\log \frac{\mathcal{Z}_{N-s}}{\mathcal{Z}_N} \sim sN\varepsilon^d \,.$$

Theorem

Consider N exchangeable hard spheres of radius ε, with zero total kinetic momentum and uniformly distributed on the energy surface corresponding to the inverse temperature β.
Then, in the limit $N \to \infty$, $\varepsilon \to 0$ with $N\varepsilon^d \to 0$, the law of s typical particles converges almost everywhere to $M_\beta^{\otimes s}$.

Entropy and chaos

A good functional to express the concentration of measure is the **entropy** defined by $S(X) = -\int f \log f$ for a random variable X of density f.

The **Shannon-Stam inequality**

$$S(\sum \lambda_i X_i) - \sum \lambda_i^2 S(X_i) \geq 0, \qquad \sum \lambda_i^2 = 1 \,.$$

provides an estimate of the entropy increase for the process of adding up independent variables, and leads to the entropic convergence towards the Gaussian (Linnik, Barron,…).

This increase may dominate the entropy loss due to local correlations, and lead to some **weak convergence of block summation** even for dependent variables (Carlen-Soffer).

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Boltzmann's approach

No need to have a precise description of the mixing properties for fixed N. **Averaging with respect to N with N>>1 should provide chaos.**

Chaos in Boltzmann's kinetic theory is **not related to time averaging** and does not require the system to be at thermodynamic equilibrium.

Boltzmann's assumption (which needs to be proved to get a rigorous derivation of kinetic theory)

$$f^{(2)}(t, z_1, z_2) \sim f^{(1)}(t, z_1) f^{(1)}(t, z_2) \,.$$

A stochastic model for the propagation of chaos

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Kac's model

Kac's stochastic process **mimics the collisions** of N hard spheres, but without transport (no spatial dependence) :

- Collision times are given by a Poisson process;
- Colliding pairs are chosen randomly;
- The law of deflection angles is given by the collision cross-section.

Kac's process is **microscopically reversible**. It is however much simpler than the deterministic dynamics as each jump is independent of the system's history.

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The mean field limit

In order that « particles exchange energy and momentum », the **mean free time** has to be O(1).

The transition probability for each pair of particles has therefore to be O(1/N).

The **mean field limit** is the dynamics

- governing the average of the empirical measure,
- obtained in the limit $N \to \infty$.

Boltzmann's equation appears then as a consequence of **the law of large numbers**.

Convergence to the Boltzmann equation

Theorem (Mischler & Mouhot)

Consider N particles initially independent and identically distributed according to some compactly supported and centered $f_0 \in L^\infty(\mathbb{R}^d)$. Then, in the mean field limit $N \to \infty$, the distribution of s typical particles $f_N^{(s)}$ converges to $f^{\otimes s}$

$$\frac{1}{s} W_1(f_N^{(s)}(t), f^{\otimes s}(t)) \to 0 \text{ as } N \to \infty,$$

where f is the solution to the homogeneous Boltzmann equation

$$\partial_t f = Q(f, f)\,,$$

on any fixed time interval $[0, T]$. Note also that the relaxation time is uniform with respect to the number N of particles.

Propagation of chaos

The rate of convergence is obtained as the sum of the initial errors (defect of factorization + empirical sampling), and the error on the generators. In particular, it requires only the **stability of the limiting equation** with respect to initial data (differentiability is defined by duality).

Assuming that the initial datum is entropically chaotic

$$\frac{1}{N} H(f_{N,0}|\gamma_N) \equiv \frac{1}{N} \int \log(f_{N,0}/\gamma_N) df_{N,0} \to H(f_0|\gamma)$$

where γ_N is the uniform probability measure on some energy surface, and γ is the Gaussian equilibrium with same energy, one has actually the **propagation of entropic chaos**.

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Dissipation

Since the functional $N^{-1}H(f_N|\gamma_N)(t)$ is monotone decreasing in time for the Markov process, one obtains directly a proof of **Boltzmann's H-theorem** in this context

$$H(f|\gamma)(t) \text{ is a non increasing function of } t\,.$$

This decay can be quantified if the **Fisher information** of the initial data is bounded

$$\int |\nabla_v \sqrt{f_0}|^2 dv < +\infty\,.$$

The propagation of chaos is therefore directly related to the **dissipation mechanism**, which has been forced by introducing randomness in the microscopic dynamics.

A deterministic result on the propagation of chaos

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Chaotic initial data

We assume that initially the hard spheres are « independent » and identically distributed

$$f_{N,0} = \frac{1}{\mathcal{Z}_N} \mathbf{1}_{\mathcal{D}_N} f_0^{\otimes N} .$$

Because of the **non overlapping condition**, independence is not satisfied for fixed radius. If $d \geq 3$, we even have

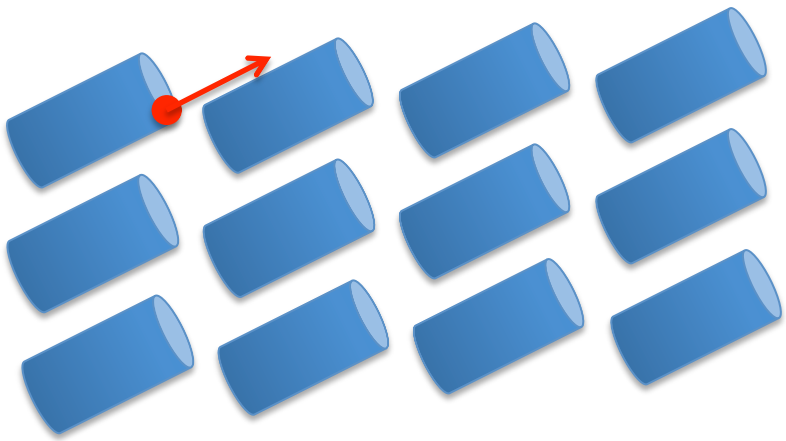
$$\mathcal{Z}_N \to 0 .$$

Independence is recovered in the limit $\varepsilon \to 0$ for any fixed marginal

$$f_{N,0}^{(s)} \to f_0^{\otimes s} .$$

The low density limit

In order that « particles exchange energy and momentum », the **mean free time** has to be O(1)



N spheres of size ε on a lattice

Volume covered by one particle of velocity v during a time t : |v|t ε

The regime for which we can observe some non trivial dynamics is the **Boltzmann-Grad scaling** $N\varepsilon^{d-1} = \alpha \sim 1$

Boltzmann's equation then comes from an **averaging over the small spatial scales.**

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Convergence to the Boltzmann equation

Theorem (Lanford)

Consider N hard spheres on $\mathbb{T}^d \times \mathbb{R}^d$ *initially "independent" and identically distributed according to* f_0

$$f_0(x,v) \leq \exp\left(-\mu - \beta \frac{|v|^2}{2}\right).$$

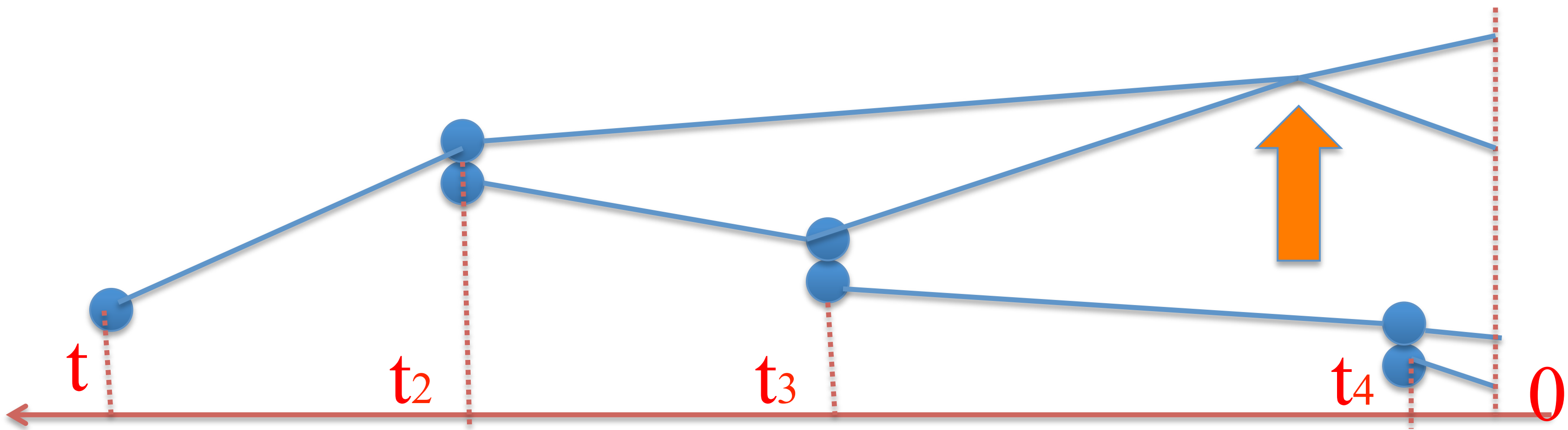
Then, in the Boltzmann-Grad limit $N \to \infty$, $\varepsilon \to 0$ *with* $N\varepsilon^{d-1} = \alpha$ *, the distribution of s typical particles* $f_N^{(s)}$ *converges almost everywhere to* $f^{\otimes s}$ *where f is the solution to the Boltzmann equation*

$$\partial_t f + v \cdot \nabla_x f = \alpha Q(f,f)$$

on a short time interval $[0, T^*(\beta,\mu)/\alpha[$.

Propagation of chaos

Solutions of the Boltzmann equation provide a good approximation as long as there is **no recollision** (i.e. no collision between two particles which are not independent)



The probability of recollisions can be estimated by a geometric argument as long as the size of collision trees remains controlled (giant components might lead to phase transition). **No such control beyond a short time.**

Fluctuations

Theorem (Bodineau, Gallagher & Saint-Raymond)

Consider N hard spheres on $\mathbb{T}^2 \times \mathbb{R}^2$ initially close to equilibrium $M_{N,\beta} = \frac{1}{\mathcal{Z}_N} \mathbf{1}_{\mathcal{D}_N} M_\beta^{\otimes N}$ with fluctuation

$$\delta f_{N,0}(x,v) = M_{N,\beta} \sum_{i=1}^{N} g_0(z_i).$$

Then, in the Boltzmann-Grad limit $N \to \infty$, $\varepsilon \to 0$ with $N\varepsilon^{d-1} = \alpha$, the fluctuation $\delta f_N^{(s)}$ converges almost everywhere to $M_\beta^{\otimes s} \sum_{i=1}^{s} g(t,z_i)$ where g is the solution to the linearized Boltzmann equation

$$\partial_t g + v \cdot \nabla_x g = \alpha \frac{2}{M} Q(M, Mg)$$

(almost) globally in time.

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Correlations and dissipation

The idea here is to kill the contribution of superexponential collision trees by using a sampling procedure together with a priori estimates coming from the **linearized entropy**

$$\int \frac{(\delta f_{N,0})^2}{M_{N,\beta}} dZ_N \leq CN \|g_0\|^2_{L^2(Mdz)} \,.$$

In particular, this provides some **control on the cumulants**, which seems to play the same role as dissipation in the Boltzmann equation.

$$N\|g_N^{(1)}(t)\|^2_{L^2(Mdz)} + \sum_{k=2}^{N} C_N^k \|g_N^{(k)}(t)\|^2_{L^2(M^{\otimes k}dZ_k)} \leq CN\|g_0\|^2_{L^2(Mdz)} \,.$$

In this strategy, chaos is prescribed initially and the dynamics seems to destroy it (at least partially).

Chaos and turbulence

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Mixing mechanisms

- Transport should introduce some mixing at small spatial scales. Physicists expect the distribution of hard spheres to be **locally Poisson at scale** $\varepsilon^{(d-1)/d}$.
- Because of this spatial randomness, the collision process should behave as a **stochastic process** mixing the velocities.
- At large spatial scales, transport is then responsible for **dispersion**. This should prevent spatial concentrations, which are the main obstacle to chaos.

Understanding the interactions of these different scales requires probably to introduce a **renormalization process**….

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